INTERNATIONAL ATOMIC ENERGY AGENCY

INDC(NDS)-0477
Distr. SZ

I N D C INTERNATIONAL NUCLEAR DATA COMMITTEE

Summary Report

First Research Coordination Meeting on

Reference Database for Neutron Activation Analysis

IAEA Headquarters
Vienna, Austria

3-5 October 2005

Prepared by

Richard B. Firestone
Lawrence Berkeley National Laboratory
University of California
Berkeley, USA

and

Andrej Trkov
IAEA Nuclear Data Section
Vienna, Austria

October 2005

Selected INDC documents may be downloaded in electronic form from http://www-nds.iaea.org/indc_sel.html or sent as an e-mail attachment. Requests for hardcopy or e-mail transmittal should be directed to services@iaeand.iaea.org or to:

Nuclear Data Section
International Atomic Energy Agency
PO Box 100
Wagramer Strasse 5
A-1400 Vienna
Austria

Produced by the IAEA in Austria
October 2005

INDC(NDS)-0477
Distr. SZ

Summary Report

First Research Coordination Meeting on

Reference Database for Neutron Activation Analysis

IAEA Headquarters
Vienna, Austria

3-5 October 2005

Prepared by

Richard B. Firestone
Lawrence Berkeley National Laboratory
University of California
Berkeley, USA

and

Andrej Trkov
IAEA Nuclear Data Section
Vienna, Austria

Abstract

Potential problems associated with nuclear data for neutron activation analysis were identified, the scope of the work to be undertaken was defined together with its priorities, and tasks were assigned to participants. Data testing and measurements refer to gamma spectrum peak evaluations, detector efficiency calibration, neutron spectrum characteristics and reference materials analysis.

October 2005

TABLE OF CONTENTS

1. Background

Due to its selectivity and sensitivity, neutron activation analysis (NAA) occupies an important place among the various analytical methods. It has proven to be a powerful non-destructive analytical technique for concentrations at or below the μg/g range, while up to 60 elements can be determined performing two irradiations and several gamma-spectrum measurements after different decay periods. The main fields of NAA application are analytical chemistry, geology, biology, and the life and environmental sciences. Its accuracy, the virtual absence of matrix effects and the completely different physical basis when compared to other analytical techniques, make it particularly suitable for the certification of candidate reference materials (RMs), providing e.g. the bulk of the literature data on the standard RMs of the National Institute of Standards and Technology and reference materials of the International Atomic Energy Agency.

The k_0 standardisation method of NAA (k_0-NAA), a concept launched in 1975, can be interpreted as an absolute standardisation method. It relies on k_0 and Q_0 factors and a few other parameters that are composite constants derived from the basic nuclear data. In practice, they are usually determined by direct measurements, partly because equivalent constants derived from the basic data are often discrepant.

The aim of the Co-ordinated Research Project (CRP) on the Reference Database for Neutron Activation Analysis is to improve the status of the database of nuclear constants for k_0-NAA, to contribute to nuclear structure and decay data and to remove or reduce some of the discrepancies that exist between the integral constants and values derived from differential data.

The INDC Committee reviews the programme of the IAEA-NDS, and has endorsed the CRP at their meeting held in May 2002. A complementary project is in progress at NAPC-Industrial Applications and Chemistry Section on "k_0-IAEA Software Development for Neutron Activation Analysis". This software package is chosen as the reference analysis tool for the current CRP.

The first Research Co-ordination Meeting (RCM) was held at the Agency Headquarters on 3-5 October 2005. The report below is a summary of the conclusions from that meeting.

2. Presentations

A. Trkov, IAEA-NDS

The objectives of the CRP were re-iterated, namely:

- to improve database of nuclear constants for k_0 NAA (improved k_0 library),
- to improve consistency between integral and differential data (activation cross-section library),
- to contribute to nuclear structure and decay data (EGAF database),
- to extend applicability of k_0 NAA.

Methods and procedures will be investigated for detector calibration, neutron spectrum characterization and gamma-spectrum processing methods. The nuclear database of integral constants will also be reviewed, performing new measurements as required.

F. De Corte, Ghent University, Belgium
A historical overview and the milestones in the most significant advances of the method were presented, explaining how the database was assembled and verified. Such information is essential for planning new measurements in order to generalize and improve the database.

R. Jaćimović, Institute Jožef Stefan, Ljubljana, Slovenia
The k_0-method was introduced at the Jožef Stefan Institute (JSI) in Ljubljana at the end of 1988. Since then all recommended procedures for applying k_0-standardization method using TRIGA Mark II reactor have been implemented. The validation of the k_0 method was established via the analysis of different reference and certified reference materials issued by the IAEA, NIST, BCR and IRMM. Up to now, relevant investigations for the CRP were done as follows: accurate determination of neutron spectrum parameters (f and α) in different irradiation channels, time-dependence of the neutron flux in different irradiation channels of the TRIGA reactor, neutron flux gradients (axial and radial) inside the irradiation channels, azimuthal variation of the neutron flux in the carousel facility (CF) of the TRIGA reactor, verification of Monte Carlo calculation of the neutron flux in CF, burn-up effects for some nuclides and systematic errors in the procedure for full-energy peak detection efficiency (ε_p) for an HPGe detector.

B. Smodiš, Institute Jožef Stefan, Ljubljana, Slovenia
Elements were identified that have incomplete information on uncertainties in their nuclear data. These should be addressed with high priority so that error propagation in routine measurements can be carried out correctly.

S.A. Jonah, Ahmadu Bello University, Nigeria
A description of the Nigerian MNSR (NIRR-1) and the experimental facilities was provided. Special mention was made of the current status of the facilities used for NAA by the relative method. In this regard, experimental procedures developed for sample analyses by the conventional method for over 30 elements were described. Measured neutron spectrum parameters required for the applicability of the k_0-standardization method were provided. The group's contribution to the CRP will be in the improvement of methodologies for determination of neutron spectrum parameters, measurement of some nuclear constants and the testing of the k_0-IAEA software.

Maria Arribere, Centro Atomico Bariloche, Argentina
The main goals of the group within this CRP are:
i) perform core modeling by using Monte Carlo techniques,
ii) perform flux characterization in the RA-6 irradiation positions through activity measurements and computational deterministic and statistical modelling,
iii) use characterized irradiation channels to perform measurements of nuclear parameters of interest in NAA using the k_0 method,
iv) use characterized irradiation channels to measure resonance integrals and thermal cross sections of isotopes where both the ground and metastable states are formed, using the methodology developed at the laboratory that has already been applied to threshold reactions.

Richard Firestone, Lawrence Berkeley National Laboratory, Berkeley CA, USA
Neutron activation analysis k_0 data will be compared with gamma-ray transition probabilities from the ENSDF and DDEP decay data files and with data from the EGAF k_0 file. New adopted decay, k_0 and cross-section data will be added into EGAF.

Zsolt Revay, KFKI, Budapest
In-beam activation technique is an excellent tool for measuring k_0 factors using pure thermal neutrons, and also for studying isotopes with short half-lives. The calculation of self-shielding is also simple in beam geometry. Moreover, when the activation is performed in a cold neutron beam, the effects of resonances disappear. A series of measurements have been started at the Prompt Gamma Activation Analysis facility of the Budapest Research Reactor to re-determine k_0 factors in the cold neutron beam. For a series of elements (like Na, Al, F, Mn), the decay peaks proved to be strong enough to analyze them in the usual prompt-gamma spectra. For weaker peaks the chopped-beam techniques is appropriate to separate the decay peaks from the prompt gamma spectrum. The elements from the priority list will be measured with either technique. The neutron spectrum was determined at the PGAA facility with time-of-flight technique using the beam chopper, and this will be done every time the beam configuration is changed. This information is used in the determination of effective g factors for nuclides such as ^{147}Gd, ^{113}Cd, etc. This project is already going on.

3. Proficiency test

The purpose of the proficiency test is to ensure that irradiation facilities and analysis software of the participants contributing experimental data will produce consistent results.

Proficiency tests will involve detector calibration, peak area determinations and neutron spectrum characterizations. Analysis will be done with k_0-IAEA software and other methods that may be available to the participants.

3.1. Gamma spectrum peak evaluation test
The coordinator for the peak evaluation test will be Menno Blaauw. He will provide standard spectra for the purpose. Participants will submit results to the coordinator who will summarize the contributions at the next meeting.

3.2. Detector efficiency calibration
The coordinator for the efficiency calibration will be Zsolt Revay. He will provide standard calibration spectra and calibration data. Participants will submit the specified results to the coordinator who will summarize the contributions at the next meeting.

3.3. Neutron spectrum characterization
The coordinator for neutron spectrum characterization will be Andrej Trkov. Monitoring material from the k_0-IAEA package will be used by all participants for spectrum characterization of their irradiation facility. In addition, Frans De Corte will provide recommendations for other candidate materials that have suitable capture and threshold reactions.

The participants will be expected to determine f and α by conventional methods. If available, participants will also provide neutron spectra in 640 group structure from statistical model

calculations or from direct measurements. Spectrum characterization results will be sent to Andrej Trkov for further analysis.

3.4. Materials analysis test

All participants will perform a materials analysis test. Frans De Corte will review the availability and appropriateness of using synthetic multi-element standard materials (SMELS) or a suitable substitute. He will also look into the future possibility of SMELS production. Maria Arribere will collect the results of the materials analysis test and write a report for the next RCM meeting.

4. k_0-IAEA software package

Recently introduced features of the k_0-IAEA software were discussed. Menno Blaauw will distribute the latest update of k_0-IAEA software to all participants.

5. Nuclear Data

Definitions of nuclear constants and their relation to differential data will also be provided by Andrej Trkov, who will also calculate a) self-shielding factors as a function of the Bondarenko dilution cross section, b) effective resonance energies and c) effective *g*-factors from the same data source.

If changes in the k_0 database are needed, all constants for a nuclide will be reviewed.

Data currently in the k_0 database will be compared with equivalent data from other sources. The purpose of this intercomparison exercises is to identify discrepant data that may require re-evaluation or new measurements.

P_γ and k_0 values will be compared and evaluated for the EGAF library by Richard Firestone. Data from the k_0 database, ENSDF, DDEP, EGAF and the literature will be considered.

Half-life data from the k_0 database provided by Frans De Corte will be compared by Mark Kellett with values from the evaluated databases.

Andrej Trkov will compare Q_0 values from the k_0 database with IRDF-2002 and JEFF-3.1 activation library.

6. Criteria for determining priorities and scope of new measurements

Priorities for re-evaluation or re-measurement of constants for the k_0 database have been elaborated as follows.

Nuclides with discrepant data

^{96}Zr	discrepant measurements of Q_0
^{94}Zr	complementary to ^{96}Zr
^{127}I	5% discrepancy in k_0
^{23}Na	different k_0 for 2 lines that should be the same

^{27}Al	2σ discrepancy between recommended and k_0 measured at KFKI
^{131}Ba	inconsistent measurements for k_0 and Q_0
^{138}Ba	inconsistent measurements for k_0 and Q_0
^{121}Sb	discrepancy in k_0, Q_0 resulting in different concentrations from 2 isotopes
^{123}Sb	discrepancy in k_0, Q_0 resulting in different concentrations from 2 isotopes

Important monitor materials
^{64}Zn
^{68}Zn

Non-1/*v* absorbers
List will be provided by Zsolt Revay.

Nuclides with high effective resonance energy E_r

Q_0	E_r	Isotope	σ_0
5.93	4300	^{90m}Y	0.001
5.05	6260	^{95}Zr	0.0499

Lower priority (Q_0<5)

1.12	2280	^{37}S	0.15
1.14	1040	^{64}Cu	2.17
1.908	2560	^{65}Zn	0.76
2.38	3540	^{75m}Ge	0.17
1.57	3540	^{75}Ge	0.34
1.8	2950	^{131}I	6.2
1.2	1540	^{143}Ce	0.95

Additional candidate materials for review will be identified by the intercomparison exercise described in Section 5. Also, Zsolt Revay will consult with Greg Kennedy whether any additional materials need to be included in the list.

There was general consensus that voluntary contributions from qualified researchers or laboratories will be valued for analysis and inclusion in the final database as appropriate. The authors will be acknowledged in the final document.

The web page is maintained by NDS for efficient exchange of information between interested parties, but is not advertised from the main web page. None of the participants objected to making the address known to potential contributors who are not formally CRP participants.

7. Next meeting

The next RCM meeting is scheduled in Spring 2007, the venue and the date to be decided.

ANNEX 1

International Atomic Energy Agency

First Research Co-ordination Meeting on

"Reference Database for Neutron Activation Analysis"

IAEA Headquarters, Vienna, Austria

3-5 October 2005

Meeting Room ACV-03-250

LIST OF PARTICIPANTS

ARGENTINA
Maria A. Arribere
Centro Atomico Bariloche
Comision Nacional de Energia Atomica
Bustillo 9500
8400 Bariloche
Rio Negro
Tel: +54 (2944) 445240
Fax: +54 (2944) 445299
E-mail: arribere@cab.cnea.gov.ar

BELGIUM
Frans De Corte
Ghent University
INW-Proeftuinstraat 86
B-9000 Gent
Tel: +32 9 2646627
Fax: +32 9 2646699
E-mail: frans.decorte@Ugent.be

HUNGARY
Zsolt Revay
Institute of Isotopes
Chemical Research Centre
Hungarian Academy of Sciences
Department of Nuclear Research
H-1121 Budapest, Konkoly Thege Str. 29-33
Tel: +36 1 392 2539
Fax: +36 1 392 2584
E-mail: revay@iki.kfki.hu

NIGERIA
Sunday A. Jonah
Centre for Energy Research and Training
(CERT)
Ahmadu Bello University
PMB 1014 Zaria
Tel: +234 69 550397
Fax: +234 69 550737
E-mail: jonahsa2001@yahoo.com

SLOVENIA
Radojko Jaćimović
Laboratory for Radiochemistry
Department of Environmental Sciences
Institute Jožef Stefan
Jamova 39
Sl-1000 Ljubljana
Tel: +386 1 5885353
Fax: +386 1 5885346
E-mail: radojko.jacimovic@ijs.si

UNITED STATES OF AMERICA
Richard B. Firestone
Lawrence Berkeley National Laboratory
University of California
1 Cyclotron Road, M/S 88RO192
Berkeley, CA 94720-8101
Tel: +1 510 486 7646
Fax: +1 510 486 5757
E-mail: RBF@lbl.gov

ADVISOR
THE NETHERLANDS
Menno Blaauw
Reactor Institute Delft
Facilities & Services Dept.
Mekelweg 15
NL-2629 JB Delft
Tel: +31 15 278 3538
Fax: +31 15 278 8430
E-mail: m.blaauw@tnw.tudelft.nl

OBSERVER
SLOVENIA
Borut Smodiš
Institute Jožef Stefan
Jamova 39
Sl-1000 Ljubljana
Tel: +386 1 2885450
E-mail: Borut.Smodis@ijs.si

IAEA:

Andrej Trkov
Nuclear Data Section
Division of Physical and Chemical Sciences
Room A2316
Tel: +43 1 2600-21712
Fax: +43 1 26007
E-mail: A.Trkov@iaea.org

Alan L. Nichols
Nuclear Data Section
Division of Physical and Chemical Sciences
Room A2313
Tel: +43 1 2600-21709
Fax: +43 1 26007
E-mail: A.Nichols@iaea.org

Mark A. Kellett
Nuclear Data Section
Division of Physical and Chemical Sciences
Room A2319
Tel: +43 1 2600 21708
Fax: +43 1 26007 21708
E-mail: M.A.Kellett@iaea.org

Matthias Rossbach
Industrial Applications and Chemistry Section
Division of Physical and Chemical Sciences
Room A2370
Tel: +43 1 2600 21750
Fax: +43 1 26007 21750
E-mail: M.Rossbach@iaea.org

Chushiro Yonezawa
Nutritional and Health Related Environmental Studies Section
Division of Human Health
Room A2424
Tel: +43 1 2600 21652
Fax: +43 1 26007 21652
E-mail: C.Yonezawa@iaea.org

ANNEX 2

International Atomic Energy Agency

First Research Coordination Meeting on

Reference Database for Neutron Activation Analysis

IAEA Headquarters, Vienna, Austria

3 – 5 October 2005

Meeting Room ACV-03-250

AGENDA

Monday, 3 October

08:30 – 09:20 **Registration** (IAEA registration desk, Gate 1)

09:30 – 10:00 **Opening Session**
Opening by Mr. N. Ramamoorthy, Director-NAPC
Introductory remarks (A.Trkov)
Election of Chairman and Rapporteur
Discussion and adoption of the Agenda (Chairman)
Election of task co-ordinators

10:00 – 11:00 *Coffee break and Administrative Matters*

11:00 – 12:20 **Session 1: Presentations by participants**
(max: 15 min per presentation + 5 min discussion)

12:20 – 14:00 *Lunch*

14:00 – 15:30 **Session 2: Presentations by participants (cont'd.)**
(max: 15 min per presentation + 5 min discussion)
General Discussion

15:30 – 16:00 *Coffee break*

16:00 – 17:30 **Session 3: Definition of a proficiency test case**
Detector calibration
Neutron spectrum determination / monitor reactions
Gamma spectrum analysis
Processing of results
General Discussion

17:30 onwards *Social event*

Tuesday, 4 October

08:30 – 09:30 **Session 4: Neutron spectrum determination**
Conventional methods of NAA
Spectrum unfolding
Direct measurements
Computational methods
General Discussion

09:30 – 10:15 **Session 5: k_0-IAEA software package**
Detector calibration utilities
Spectrum processing utilities
Scope of software intercomparison with other products
Software extensions
General Discussion

10:15 – 10:45 *Coffee break*

10:45 – 12:15 **Session 6: Specific features**
Items drafted by chairman

12:15 – 14:00 *Lunch*

14:00 – 15:30 **Session 7: Nuclear constants in relation to differential data**
Relation between integral and differential data
Neutron self-shielding
Effective resonance energy
Gamma emission probabilities

15:30 – 16:00 *Coffee break*

16:00 – 17:30 **Session 8: Criteria for determining the scope of new measurements**
Needs and priorities
Available facilities
Available manpower

Wednesday, 5 October

08:30 – 10:15 **Session 9: Task assignment and drafting of summary report**

10:15 – 10:45 *Coffee break*

10:45 – 12:15 **Session 10: Task assignment and drafting of summary report**

12:15 – 14:00 *Lunch*

14:00 – 15:30 **Session 11:Review of the summary report**

15:30 **Closing of the meeting**

GUIDELINES

General:

- Please, check the NAA CRP web page http://www-nds.iaea.org/naa/index.html frequently for announcements and up-to-date information.
- For all administrative queries please contact Ms. Janet Roberts on J.Roberts@iaea.org.
- For technical matters please contact the technical officer of the project Andrej Trkov on A.Trkov@iaea.org. with a copy to Ms. Roberts.

Presentations:

- Oral presentations at the meeting are deliberately short.
- The presentations should *not* describe details of the theoretical advances, but primarily inform other participants (not necessarily experts in the specific field) on your planned contribution to the CRP.

ANNEX 3

TASK ASSIGNMENTS

Participant	Date	Task	Status
		Gamma spectrum peak evaluation test.	
Menno Blaauw	11 July 2006	Coordinate activity.	
	5 Dec. 2005	Provide standard spectra for purpose to participants.	
All participants	30 April 2006	Submit results to coordinator.	
Menno Blaauw	Next RCM	Summarize contributions.	
		Detector efficiency calibration.	
Zsolt Revay	May 2006	Coordinate activity. Provide standard calibration spectra and calibration data to participants.	
All participants	31 Oct 2006	Submit results according to specifications to coordinator.	
Zsolt Revay	Next RCM	Summarize contributions.	
		Neutron spectrum characterization.	
Andrej Trkov	Next RCM	Coordinate activity.	
Frans De Corte	Dec. 2005	Provide recommendations for other candidate materials that have suitable capture and threshold reactions.	Done
All participants	Dec. 2006	Monitoring material from the k_0-IAEA package to be used by all participants for spectrum characterization of their irradiation facility, in addition to any other available monitor materials. Determine f and α by conventional methods.	
All participants	Dec. 2006	If available, also provide neutron spectra in 640 group structure from statistical model calculations or from direct measurements. To be sent to Andrej Trkov for further analysis.	
Andrej Trkov	Next RCM	Further analysis of spectrum characterization results.	
Andrej Trkov	Next RCM	Summarize contributions.	
		Materials analysis test.	
Maria Arribere	Next RCM	Coordinate activity.	
All participants	Next RCM	To perform a materials analysis test.	

Participant	Date	Task	Status
		Materials analysis test (cont.).	
Frans De Corte	Dec. 2005	To review the availability and appropriateness of using synthetic multi-element standard materials (SMELS) or a suitable substitute. To look into the future possibility of SMELS production.	Done
Maria Arribere	Next RCM	Collect the results and write a report.	
		k_0-IAEA software package.	
Menno Blaauw	12 Dec 2005	Distribute the latest update of k_0-IAEA software to all participants.	
		Nuclear Data	
Andrej Trkov	7 Jan 2006	Provide definitions of nuclear constants and their relation to differential data. Calculate a) self-shielding factors as a function of the Bondarenko dilution cross section, b) effective resonance energies and c) effective *g*-factors from the same data source.	
	Sept. 2006	Data currently in the k_0 database to be intercompared with equivalent data from other sources to identify discrepant data that may require re-evaluation or new measurements	
Richard Firestone	Dec. 2006	Compare and evaluate P_γ and k_0 values for the EGAF library. Data from the k_0 database, ENSDF, DDEP, EGAF, and the literature to be considered.	
Frans De Corte	Oct. 2005	Provide half-life data from the k_0 database.	Done
Mark Kellett	Jan. 2006	Compare half-life data from the k_0 database with values from the evaluated databases.	
		Criteria for determining priorities and scope of new measurements.	
Zsolt Revay	28 Feb. 2006	Consult with Greg Kennedy whether any additional materials need to be included in the list.	

Nuclear Data Section
International Atomic Energy Agency
P.O. Box 100
A-1400 Vienna
Austria

e-mail: services@iaeand.iaea.org
fax: (43-1) 26007
cable: INATOM VIENNA
telex: 1-12645
telephone: (43-1) 2600-21710